Chem 20AH

1st MIDTERM, October 25, 2017

NAME______________________________

Problem	Points possible	Points scored
1(a)	15	
1(b)	15	
2 (a)	10	
2 (b)	10	
3(a)	10	
3(b)	10	
3(c)	5	
4(a)	10	
4(b)	10	
4(c)	5	
	100	

BE SURE TO SHOW ALL YOUR WORK, I.E., MAKE CLEAR THE REASONING BEHIND YOUR SOLUTION TO EACH PROBLEM.

BE CAREFUL TO WRITE UNITS FOR EVERY QUANTITY WITH DIMENSIONS, WITHOUT EXCEPTION.

A PERIODIC TABLE, A LIST OF FUNDAMENTAL CONSTANTS, AND SOME POSSIBLY USEFUL EQUATIONS, ARE PROVIDED ON THE LAST PAGE OF THE EXAM.

+15

1. (30 points)

(a) (15 points) Butane (C4H10) gas reacts with oxygen (O2) gas to give carbon dioxide (CO2) gas and water vapor (H20). For every 1g of butane that reacts, how many grams of water vapor are produced?

Balanced eq.: $2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$ (based on atomic theory & law of conservation of matter)

Molar mass of C_4H_{10}: $4(12.01 \frac{g}{mol}) + 10(1.01 \frac{g}{mol}) = 58.14 \frac{g}{mol}$

" of H_2O: $2(1.01 \frac{g}{mol}) + 16.00 \frac{g}{mol} = 18.02 \frac{g}{mol}$

$$1 \text{ g } \cancel{C_4H_{10}} \cdot \frac{1 \cancel{\text{mol } C_4H_{10}}}{58.14 \text{ g } \cancel{C_4H_{10}}} \cdot \frac{10 \cancel{\text{mol } H_2O}}{2 \cancel{\text{mol } C_4H_{10}}} \cdot \frac{18.02 \text{ g } H_2O}{1 \cancel{\text{mol } H_2O}} = \boxed{1.550 \text{ g } H_2O} \text{ produced}$$

(assume "exactly" 1 gram... or highly precisely)

since 2 moles of C_4H_{10} reacts completely w/ O_2 to form 10 moles H_2O, according to the balanced equation

+15

(b) (15 points) If 11g of butane and 21g of oxygen are present initially, what amounts of each reactant and product are present when the reaction goes to completion?

$$11 \text{ g } \cancel{C_4H_{10}} \cdot \frac{1 \text{ mol } C_4H_{10}}{58.14 \text{ g } \cancel{C_4H_{10}}} = 0.19 \text{ mol } C_4H_{10}$$

$$21 \text{ g } \cancel{O_2} \cdot \frac{1 \text{ mol } O_2}{32.00 \text{ g } \cancel{O_2}} = 0.66 \text{ mol } O_2$$

present initially

0.66 mol O_2 reacts with only $0.66 \text{ mol}\left(\frac{2}{13}\right) = 0.10$ mol C_4H_{10}, so it is the limiting reactant — and those are the amounts that react, leaving 0.19 mol − 0.10 mol = 0.09 mol excess unreacted C_4H_{10}.

For the products:

$$0.66 \cancel{\text{mol } O_2} \cdot \frac{8 \text{ mol } CO_2}{13 \cancel{\text{mol } O_2}} = 0.41 \text{ mol } CO_2$$

$$0.66 \cancel{\text{mol } O_2} \cdot \frac{10 \text{ mol } H_2O}{13 \cancel{\text{mol } O_2}} = 0.51 \text{ mol } H_2O$$

Final Quantities

0 mol O_2
0.09 mol C_4H_{10}] R
0.41 mol CO_2
0.51 mol H_2O] P

+30

2. (20 points)
According to the Bohr theory of hydrogen-like (i.e., single-electron) atomic species, *the radii of the electron orbits are quantized* according to

$$r = a_o \frac{n^2}{Z},\ n = 1,2,3,\ldots$$

where $a_o = \frac{\varepsilon_o h^2}{\pi e^2 m_e} = 0.53$ Å is "the Bohr radius".

(a) (10 points) Use these results in the potential energy (of interaction between the electron and nucleus) $-\frac{Ze^2}{4\pi\varepsilon_o r}$ to obtain *the quantized values of the potential energy* (PE).

Simply substitute the quantized expression for r to get the corresponding potential energies (which are thus quantized).

$$PE_n = -\frac{Ze^2}{4\pi\varepsilon_o a_o \frac{n^2}{Z}} = -\frac{Z^2e^2}{4\pi\varepsilon_o a_o n^2} = \boxed{-\frac{e^2}{4\pi\varepsilon_o a_o}\cdot\frac{Z^2}{n^2}} \quad n = 1,2,3,\ldots$$

Why not substitute in a_o too?

Don't know

$$= -\frac{e^2}{4\pi\varepsilon_o\left(\frac{\varepsilon_o h^2}{\pi e^2 m_e}\right)}\cdot\frac{Z^2}{n^2} = -\frac{\pi e^4 m_e}{4\pi\varepsilon_o^2 h^2}\cdot\frac{Z^2}{n^2} = \boxed{-\frac{e^4 m_e}{4\varepsilon_o^2 h^2}\cdot\frac{Z^2}{n^2}} \quad n = 1,2,3,\ldots$$

10 pts

(b) (10 points) In part (a) above you should have found a result for the PE that differs only by a numerical factor from the familiar quantized values of the *total* energy, $E_n = -\frac{1}{8}\frac{Z^2 m_e e^4}{\varepsilon_o^2 h^2}\frac{1}{n^2}$, $n = 1, 2, 3, \ldots$, for a one-electron *Z*-atom. Use this result for the PE – or the expression for the quantized total energy – to calculate the ratio of the ionization energy of Li^{++} to that of H.

IE of Li^{++}: $\quad Li^{++} \rightarrow Li^{3+} + e^- \quad \Delta E = IE = E_f - E_i$

$$= 0 - E_1 = -\left(-\frac{1}{8}\frac{3^2 m_e e^4}{\varepsilon_o^2 h^2}\frac{1}{n^2}\right) = 9\,\frac{m_e e^4}{8\varepsilon_o^2 h^2}\frac{1}{n^2}$$

10 pts

IE of H: $\quad H \rightarrow H^+ + e^- \quad \Delta E = IE = E_f - E_i$

$$= 0 - E_1 = -\left(-\frac{1}{8}\frac{1^2 m_e e^4}{\varepsilon_o^2 h^2}\frac{1}{n^2}\right) = 1\,\frac{m_e e^4}{8\varepsilon_o^2 h^2}\frac{1}{n^2}$$

because no electrostatic force between p^+ and e^- if no e^- are present.?

$$\frac{IE_{Li^{++}}}{IE_H} = \boxed{9}$$

3. (25 points) Consider the ionic bond of the AB molecule, in which A is the more electronegative atom. Suppose its measured bond length R_e is 1.9Å, and its measured dipole moment is 4.4 Debye.

(a) (10 points) What is the effective charge on each atom?

high IE → hard to lose e⁻
high EA → gains much from adding e⁻

– A should be negatively charged since it is more electronegative (and B should be positively charged).

Dipole Moment:

$\mu = q \cdot R_e$ ⟶ $q = \frac{\mu}{R_e} = \frac{4.4\,D}{1.9\,Å} = \frac{4.4(3.336 \cdot 10^{-30}\,C \cdot m)}{1.9 \cdot 10^{-10}\,m} = 7.7 \cdot 10^{-20}\,C$

$q = \delta$ (1 unit of charge) → $0.48 \cdot e$

10

Atom A: $\boxed{-7.7 \cdot 10^{-20}\,C}$ or $-0.48\,e$

Atom B: $\boxed{7.7 \cdot 10^{-20}\,C}$ or $0.48\,e$

(b) (10 points) In the case of an AB bond that is 100% ionic, the effective charges on *A* and *B* are $-e$ and $+e$, respectively, and the electrostatic energy of attraction between the A^- and B^+ atomic species is $\boxed{-\frac{e^2}{4\pi\varepsilon_0 R_e}}$. But to finish an estimate of the bond energy you would need to calculate the net energy required to create the independent A^- and B^+ ions. Write this net energy – to form the singly-charged ions A^- and B^+ from the neutral atoms *A* and *B* – in terms of the ionization energies (IE_A and/or IE_B) and electron affinities (EA_A and/or EA_B) of the *A* and *B* atoms.

$B \rightarrow B^+ + e^-$ $\quad \Delta E_1 = IE_B$

$A + e^- \rightarrow A^-$ $\quad \Delta E_2 = -EA_A$

Net energy (to create ions A^- and B^+) $= \Delta E_1 + \Delta E_2 = \boxed{IE_B - EA_A}$

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(c) (5 points). If the electron affinity of *A* is 328 kJ/mole, what is the ionization energy of A^-?

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$A + e^- \rightarrow A^-$ $\quad \Delta E = -EA = -328$ kJ/mol

Now simply reverse: energy that's released becomes energy required

$A^- \rightarrow A + e^-$ $\quad \Delta E = \boxed{328\text{ kJ/mol}}$

(This is the IE of A^-!)

4) (25 points) The lowest-energy state of a particle in a box of length L centered at $x=L/2$ has normalized wavefunctions given by $\psi_n(x)=\sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$.

(a) (10points) By substituting $\psi_3(x)=\sqrt{\frac{2}{L}}\sin(\frac{3\pi x}{L})$ into the Schrodinger equation for the particle in a box, i.e., $-\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2}\psi(x)=E\psi(x)$, determine the energy corresponding to this state.

$$\frac{d^2}{dx^2}\psi_3(x)=\frac{d}{dx}\left(\sqrt{\frac{2}{L}}\cdot\frac{3\pi}{L}\cos\left(\frac{3\pi x}{L}\right)\right)=\sqrt{\frac{2}{L}}\cdot\left(\frac{3\pi}{L}\right)^2\cdot-\sin\left(\frac{3\pi x}{L}\right)$$

$$=-\left(\frac{3\pi}{L}\right)^2\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)=\boxed{-\left(\frac{3\pi}{L}\right)^2\psi_3(x)}$$ → substitute into the equation...

$$-\frac{h^2}{8\pi^2 m}\left(-\left(\frac{3\pi}{L}\right)^2\right)\psi_3(x)=E\psi_3(x)$$

$$E=\frac{h^2}{8\pi^2 m}\cdot\frac{9\pi^2}{L^2}=\boxed{\frac{9h^2}{8mL^2}}$$ energy corresponding to $n=3$ state of p-in-a-b

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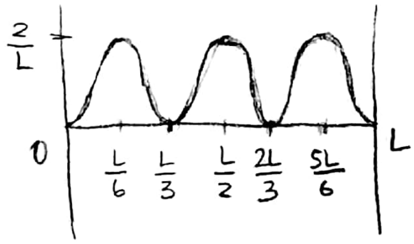
(b) (10 points). Plot the square of $\psi_3(x)=\sqrt{\frac{2}{L}}\sin(\frac{3\pi x}{L})$, showing where it has its maxima (and indicate its values there), and also show where it vanishes (i.e., where it equals zero).

$$\psi_3^2(x)=\frac{2}{L}\sin^2\left(\frac{3\pi}{L}x\right)$$



Maxima at $\boxed{\frac{L}{6},\ \frac{L}{2}\text{ and }\frac{5L}{6}}$

where $\psi_3^2(x)=\frac{2}{L}$. (since $\sin^2 x$ has range $0\to1$)

Vanishes at $\boxed{0,\ \frac{L}{3},\ \frac{2L}{3}\text{ and }L}$

where $\psi_3^2(x)=0$. Particle cannot exist there!

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(c) (5 points). What is the probability of finding the particle in the middle third of the box (i.e., between $x=\frac{1}{3}L$ and $x=\frac{2}{3}L$, when it is in the state ψ_3?

According to the graph for ψ_3, the particle has equal probabilities of being in the first, middle, and last third of the box.

Thus the probability of being in the middle third is $\boxed{\frac{1}{3}}$. (All Probabilities sum to 1.)

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SOME USEFUL INFORMATION

PERIODIC TABLE (or, at least, the first 54 elements of it…) – please use only the appropriate number of significant figures for each atomic weight.

Key: 11 — Atomic number; Na — Element symbol; Sodium — Element name; 22.99 — Average atomic mass*

	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	
1 **H** Hydrogen 1.01																	2 **He** Helium 4.00
3 **Li** Lithium 6.94	4 **Be** Beryllium 9.01											5 **B** Boron 10.81	6 **C** Carbon 12.01	7 **N** Nitrogen 14.01	8 **O** Oxygen 16.00	9 **F** Fluorine 19.00	10 **Ne** Neon 20.18
11 **Na** Sodium 22.99	12 **Mg** Magnesium 24.31											13 **Al** Aluminum 26.98	14 **Si** Silicon 28.09	15 **P** Phosphorus 30.97	16 **S** Sulfur 32.07	17 **Cl** Chlorine 35.45	18 **Ar** Argon 39.95
19 **K** Potassium 39.10	20 **Ca** Calcium 40.08	21 **Sc** Scandium 44.96	22 **Ti** Titanium 47.87	23 **V** Vanadium 50.94	24 **Cr** Chromium 52.00	25 **Mn** Manganese 54.94	26 **Fe** Iron 55.85	27 **Co** Cobalt 58.93	28 **Ni** Nickel 58.69	29 **Cu** Copper 63.55	30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.72	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.92	34 **Se** Selenium 78.96	35 **Br** Bromine 79.90	36 **Kr** Krypton 83.80
37 **Rb** Rubidium 85.47	38 **Sr** Strontium 87.62	39 **Y** Yttrium 88.91	40 **Zr** Zirconium 91.22	41 **Nb** Niobium 92.91	42 **Mo** Molybdenum 95.94	43 **Tc** Technetium (98)	44 **Ru** Ruthenium 101.07	45 **Rh** Rhodium 102.91	46 **Pd** Palladium 106.42	47 **Ag** Silver 107.87	48 **Cd** Cadmium 112.41	49 **In** Indium 114.82	50 **Sn** Tin 118.71	51 **Sb** Antimony 121.76	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90	54 **Xe** Xenon 131.29

Some assorted constants, and facts…:

$N_{Avogadro} = 6.02 \times 10^{23}$/mole

1 ev = 1.60×10^{-19} Joule (J)

1 kJ = 10^3 J

1 Debye (D) = 3.336×10^{-30} C m

$e = 1.60 \times 10^{-19}$ C

1Å= 10^{-10}m

$\varepsilon_o = 8.85 \times 10^{-12}\ C^2\ J^{-1}\ m^{-1}$

$h = 6.63 \times 10^{-34}$ J s

$\nu = \frac{c}{\lambda}$

$E = h\nu$, for energy carried by light of frequency ν

$V = \frac{q_1 q_2}{4\pi\varepsilon_o r}$ is the potential energy of two charges separated by a distance r

$F = \frac{q_1 q_2}{4\pi\varepsilon_o r^2}$ is the corresponding force

$\mu = q \cdot R_e$ is the dipole moment of a bond, where R_e is the length of the bond and q is the charge transferred from one atom to the other when the bond is formed.

Ryd= Rydberg constant $= \frac{m_e e^4}{8\varepsilon_o^2 h^2}$ = 13.6 ev

Exact quantum mechanical energies for a one-electron atomic species: $E_n = -\frac{Z^2}{n^2} Ryd$

$$\frac{d}{dx}\sin(u(x)) = \cos(u(x)) \cdot \frac{du(x)}{dx}$$

$$\frac{d}{dx}\cos(u(x)) = -\sin(u(x)) \cdot \frac{du(x)}{dx}$$